Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-
26946-56-5 | DTXSID10447169

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -5.12 °C

Global applicability domain: Inside

Local applicability domain index: 6.18e-01

Confidence level: 5.35e-01

Nearest Neighbors from the Training Set

Image not found
Sebacil
Measured: 40.5
Predicted: 16.6

Image not found
1,2-Cycloheptanedione
Measured: -40.0
Predicted: -14.4

Image not found
Allethrin
Measured: -40.0
Predicted: -20.4

Image not found
Methyl dihydrojasmonate
Measured: -10.0
Predicted: -2.67

Image not found
2-Oxetanone, 3,3-dimethyl-4-(1-methylethylidene)- (9CI)
Measured: -18.0
Predicted: -16.5